

Flux Phase in Bilayer $t - J$ Model

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Various experiments suggest that time-reversal symmetry (\mathcal{T}) is broken spontaneously in some of the high- T_C cuprate superconductors.¹⁻⁴⁾ For example, Covington *et al.*¹⁾ observed the peak splitting of zero bias conductance in ab-oriented YBCO/insulator/Cu junctions. This has been interpreted as a sign of \mathcal{T} violation caused by the introduction of superconducting (SC) order parameter (OP) with a symmetry different from that in the bulk.⁵⁻⁷⁾ In this case, spontaneous currents would flow along the surface, and a magnetic field should be generated locally. However, experimental evidence for such magnetic fields is still controversial.^{8,9)}

Recently, the present author has studied the (110) surface state of high- T_C cuprate superconductors based on the Bogoliubov de Gennes (BdG) method applied to a single-layer $t - J$ model, and it was found that the flux phase can occur as a surface state.^{10,11)} The flux phase is a mean-field (MF) solution to the $t - J$ model in which staggered currents flow and the flux penetrates the plaquette in a square lattice, but it is unstable toward the $d_{x^2-y^2}$ -wave SC instability.¹²⁻¹⁶⁾ (The d -density wave states, which have been introduced in a different context, have similar properties.¹⁷⁾) Near the (110) surfaces, the $d_{x^2-y^2}$ -wave SC order is strongly suppressed and then the flux phase that is forbidden in the bulk may arise.¹¹⁾ Once it occurs, the spontaneous currents flow along the surface, leading to local \mathcal{T} violation. However, the doping range in which \mathcal{T} violation arises was much narrower than that observed experimentally in YBCO, if we use an effective single-layer model.¹⁸⁾

In this short note, we study the bare transition temperature of the flux phase (assuming the absence of SC order), T_{FL} , in a bilayer $t - J$ model that describes the electronic states of the YBCO system more accurately. The critical doping rate δ_c , at which T_{FL} vanishes, is estimated and compared with that in the single-layer model. In

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bilayer models, there may be two types of flux phase, *i.e.*, the directions of the flux in two layers are the same or opposite. When the latter state arises, the magnetic fields generated in two layers cancel each other.

We consider the bilayer $t - J$ model on a square lattice whose Hamiltonian is given by $H = H_1 + H_2 + H_\perp$ with

$$H_i = - \sum_{j,\ell,\sigma} t_{j\ell} \tilde{c}_{j\sigma}^{(i)\dagger} \tilde{c}_{\ell\sigma}^{(i)} + J \sum_{\langle j,\ell \rangle} \mathbf{S}_j^{(i)} \cdot \mathbf{S}_\ell^{(i)}, \quad (i = 1, 2) \quad (1)$$

$$H_\perp = - \sum_{j,\ell,\sigma} t_{j\ell}^\perp \left(\tilde{c}_{j\sigma}^{(1)\dagger} \tilde{c}_{\ell\sigma}^{(2)} + h.c. \right) + J_\perp \sum_j \mathbf{S}_j^{(1)} \cdot \mathbf{S}_j^{(2)}, \quad (2)$$

where the transfer integrals (in plane) $t_{j\ell}$ are finite for the first- (t), second- (t'), and third-nearest-neighbor bonds (t''), or zero otherwise. J (J_\perp) is the intraplane (inter-plane) antiferromagnetic superexchange interaction, and $\langle j, \ell \rangle$ denotes nearest-neighbor bonds. The interplane transfer integrals $t_{j\ell}^\perp$ are chosen to reproduce the dispersion in k space,¹⁹⁾ $t_k^\perp = -t_0^\perp (\cos k_x - \cos k_y)^2$, namely, "on-site" (t_0^\perp), second- ($t_2^\perp = -t_0^\perp/2$), and third-nearest-neighbor bonds ($t_3^\perp = t_0^\perp/4$) are taken into account.

$\tilde{c}_{j\sigma}^{(i)}$ is the electron operator for the i -th layer ($i = 1, 2$) in Fock space without double occupancy. We treat this condition using the slave-boson MF theory.^{10, 11, 14, 20–22)} Although the bosons are not condensed in purely two-dimensional systems at a finite temperature (T), they are almost condensed at a low T (*i.e.*, $T < 3J/16$ where the flux phase may occur) and for finite carrier doping ($\delta \gtrsim 0.05$). Then, we treat them as Bose-condensed. (For a small δ , the absence of Bose condensation may lead to a flux phase as a stable solution.^{14, 16)}) This procedure amounts to renormalizing the transfer integrals by multiplying δ (δ being the doping rate), *e.g.*, $t \rightarrow t\delta$, *etc.*, and rewriting $\tilde{c}_{j\sigma}$ as $f_{j\sigma}$. In a qualitative sense, this approach is equivalent to the renormalized mean-field theory of Zhang *et al.*²³⁾ (Gutzwiller approximation).

We decouple the Hamiltonian by dividing the system into two sublattices A and B. The bond OPs may be complex numbers when the flux order occurs, and we define intralayer OPs as $\sum_\sigma \langle f_{j\sigma}^{(i)\dagger} f_{j+\hat{x}\sigma}^{(i)} \rangle \equiv x_s + i(-1)^{j_x+j_y} y_s$, $\sum_\sigma \langle f_{j\sigma}^{(i)\dagger} f_{j+\hat{y}\sigma}^{(i)} \rangle \equiv x_s - i(-1)^{j_x+j_y} y_s$. Here, \hat{x} (\hat{y}) is a unit vector in the x (y)-direction (the lattice constant is taken to be unity), and x_s and y_s are real constants. For interlayer bonds, we define $\sum_\sigma \langle f_{j\sigma}^{(1)\dagger} f_{j\sigma}^{(2)} \rangle \equiv x_s^\perp$, with x_s^\perp being a real constant. Now we note that there are two ways of coupling the layers; a site in the A sublattice in one layer may be on top of a site in the A (or B) sublattice of the other layer. We call the former (latter) one as a type A (B) flux phase.

Energy eigenvalues are obtained by diagonalizing the Hamiltonian. They are given

as $E_k^{(\alpha\beta)} = \alpha|\xi_k| + \beta\epsilon_k^\perp + \epsilon_k$ for the type A, $E_k^{(\alpha\beta)} = \alpha|\xi_k + \beta\epsilon_k^\perp| + \epsilon_k$ for the type B flux phase, respectively, with $\alpha, \beta = \pm$. Here, $\text{Re } \xi_k = -(2t\delta + 3Jx_s/4)(\cos k_x + \cos k_y)$, $\text{Im } \xi_k = -3Jy_s/4(\cos k_x - \cos k_y)$, $\epsilon_k = -\mu - 4t'\delta \cos k_x \cos k_y - 2t''\delta(\cos 2k_x + \cos 2k_y)$, $\epsilon_k^\perp = t_k^\perp \delta - 3J_\perp x_s^\perp/8$, and μ is the chemical potential. Free energy can be calculated using $E_k^{(\alpha\beta)}$,

$$F_{MF} = E_0 - 2T \sum_{\alpha, \beta = \pm, k} \log[1 + \exp(-E_k^{(\alpha\beta)}/T)] + 2\mu N(1 - \delta), \quad (3)$$

where summation on k is taken over the region $|k_x| + |k_y| \leq \pi$, and $E_0 = N[\frac{3J}{2}(x_s^2 + y_s^2) + \frac{3J_\perp}{8}(x_s^\perp)^2]$ with N being the total number of lattice sites within a plane. Self-consistency equations for the OPs and the chemical potential can be obtained by varying the free energy F_{MF} ,^{10,14)} and we solve them numerically.

T_{FL} corresponding to the YBCO system is shown in Fig. 1. Here, the band parameters are chosen after Ref. 24; $t/J = 2.5$, $t'/t = -0.3$, $t''/t = 0.15$, $t_0^\perp/t = 0.15$, and $J_\perp/J = 0.1$. These parameters were chosen to reproduce experimental results for YBCO.²⁴⁾ It is seen that the T_{FL} for the type B flux phase is higher than that of the type A flux phase for $\delta \lesssim 0.15$. The critical doping rate for the type A (B) flux phase is $\delta_c \sim 0.190$ (0.152). Thus, δ_c in the bilayer model is consistent with that obtained in the experiment.¹⁾ At high doping rates, the T_{FL} for the type B flux phase shows a reentrant behavior at a low T as in the case of the single-layer model. This is because the nesting condition for the Fermi surface is changed for a large δ , and then the incommensurate flux order, which is not taken into account in the present work, will be more favorable. For comparison, we also calculate the SC transition temperature T_C , using the self-consistency equations Eqs. (12)-(14) in Ref. 24. As seen, T_C is always higher than T_{FL} at any finite δ , so that the stable solution in the bulk is the SC state.

For comparison, we present the results for $t_0^\perp = J_\perp = 0$ in Fig. 2. T_{FL1} (T_{FL2}) is that for $t/J = 2.5$ and $t' = t'' = 0$ ($t/J = 2.5$, $t'/t = -0.3$, and $t''/t = 0.15$), and the corresponding SC transition temperature T_{C1} (T_{C2}) is also shown. It is seen that δ_c is larger than that in Ref. 11, *i.e.*, $\delta_c \sim 0.11$ (0.08) for $t/J = 4$ and $t' = t'' = 0$ ($t/J = 4$, $t'/t = -1/5$, and $t''/t = 1/6$, corresponding to the YBCO-type Fermi surface). This means that the larger J/t is mainly responsible for the larger δ_c , although the bilayer couplings (and also t' and t'') may also affect it.

Near a (110) surface, the $d_{x^2-y^2}$ -wave SC order is strongly suppressed, and the flux phase would occur as in the single-layer model, with currents flowing along the sur-

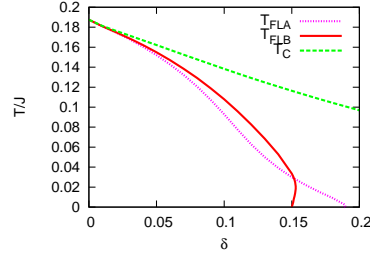


Fig. 1. (Color online) Bare transition temperature of the flux phase of Type A (T_{FLA}), type B (T_{FLB}), and superconductivity (T_C). See text for details.

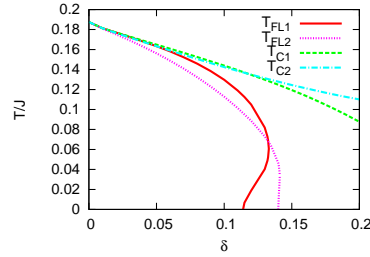


Fig. 2. (Color online) Bare transition temperature of the flux phase, T_{FL} , and superconductivity, T_C , without interlayer couplings. See text for details.

face.¹¹⁾ In the type B flux phase, the current on the different layers will flow in opposite directions, and the magnetic field generated by these currents would vanish macroscopically. This may explain why no magnetic field is observed in some experiments for the (110) surface of YBCO.⁹⁾

In the single-layer model, the doping range where the flux phase exists is larger in inhomogeneous systems than in uniform systems, because the incommensurate order not taken into account in the latter is expected in the former.¹¹⁾ We can expect that it is also the case in bilayer systems. Whether the transition from type B to A surface flux states (*i.e.*, appearance of the local magnetic field near the surface) indeed occurs with increasing δ will be examined by BdG calculations. The local density of states should also be investigated to determine whether the peak splitting of zero bias conductance without a macroscopic magnetic field may be possible. These problems will be studied separately.

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References

- 1) M. Covington, M. Aprili, E. Paraoanu, L. H. Greene, F. Xu, J. Zhu, and C. A. Mirkin, Phys. Rev. Lett. **79**, 277 (1997).
- 2) J. Xia, E. Schemm, G. Deutscher, S. A. Kivelson, D. A. Bonn, W. N. Hardy, R. Liang, W. Siemons, G. Koster, M. M. Fejer, and A. Kapitulnik, Phys. Rev. Lett. **100**, 127002 (2008).
- 3) H. Karapetyan, M. Hücker, G. D. Gu, J. M. Tranquada, M. M. Fejer, J. Xia, and A. Kapitulnik, Phys. Rev. Lett. **109**, 147001 (2012).
- 4) H. Karapetyan, J. Xia, M. Hücker, G. D. Gu, J. M. Tranquada, M. M. Fejer, and A. Kapitulnik, Phys. Rev. Lett. **112**, 047003 (2014).
- 5) M. Fogelström, D. Rainer, and J. A. Sauls, Phys. Rev. Lett. **79**, 281 (1997).
- 6) M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn. **64**, 3384 (1995).
- 7) M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn. **64**, 4867 (1995).
- 8) R. Carmi, E. Polturak, G. Koren, and A. Auerbach, Nature **404**, 853 (2000).
- 9) H. Saadaoui, Z. Salman, T. Prokscha, A. Suter, H. Huhtinen, P. Paturi, and E. Morenzoni, Phys. Rev. B **88**, 180501(R) (2013).
- 10) K. Kuboki, J. Phys. Soc. Jpn. **83**, 015003 (2014).
- 11) K. Kuboki, J. Phys. Soc. Jpn. **83**, 054703 (2014).
- 12) I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988).
- 13) F. C. Zhang, Phys. Rev. Lett. **64**, 974 (1990).
- 14) K. Hamada and D. Yoshioka, Phys. Rev. B **67**, 184503 (2003).
- 15) M. Bejas, A. Greco, and H. Yamase, Phys. Rev. B **86**, 224509 (2012).
- 16) H. Zhao and J. R. Engelbrecht, Phys. Rev. B **71**, 054508 (2005).
- 17) S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 094503 (2001).
- 18) T. Tanamoto, H. Kohno, and H. Fukuyama, J. Phys. Soc. Jpn. **61**, 1886 (1992).
- 19) O. K. Andersen, A. I. Lichtenstein, O. Jepsen, and F. Paulsen, J. Phys. Chem. Solids **56**, 1573 (1995).
- 20) Z. Zou and P. W. Anderson, Phys. Rev. B **37**, 627 (1988).

- 21) For a review on the $t - J$ model, see M. Ogata and H. Fukuyama, Rep. Prog. Phys. **71**, 036501 (2008).
- 22) P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. **78**, 17 (2006).
- 23) F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. **1**, 36 (1988).
- 24) H. Yamase and W. Metzner, Phys. Rev. B **73**, 214517 (2006).